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EVAPORATION DYNAMICS OF A SEVEN-COMPONENT MIXTURE CONTAINING NERVE AGENT SIMULANTS

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14. ABSTRACT
This report evaluates the effect of low-volatility components on the volatility of dimethyl methylphosphonate (DMMP). Experimentation utilizes measurements of pure DMMP, comparing those results to mixtures as a function of concentration and time.

15. SUBJECT TERMS

Evaporation rate	Dimethyl methylphosphonate	Propyl ether
Dimethyl hydrogen phosphonate	Phosphoric acid	DMMP

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EXECUTIVE SUMMARY

This report summarizes experiments to measure the evaporation of dimethyl methylphosphonate (DMMP) in a mixture containing six other compounds. The expected result is an increase in DMMP volatility in proportion with its mole fraction in the mixture owing to loss of more volatile components, that is, di-(n-propyl) ether (PE) and dimethyl hydrogen phosphonate (DMHP).

Experimentation utilized the saturator cell approach to generate a stream composed of carrier gas and a mixture of the volatile components of the seven-component mixture. Analysis of the resulting effluent stream mixtures was performed using mass spectrometry (MS) and gas chromatography (GC) with flame ionization detection (FID). MS, GC and FID were also used for identification and quantification of each species in the mixture as a function of time.

The evaporation dynamics of the volatile components of the seven-component mixture indicated that the PE component does not behave ideally, while the DMMP and DMHP behave as expected based on Raoult's Law.

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PREFACE

The work described in this report was authorized under Project No. ECBC/CAPP/6.1. The work began in October 2010 and completed in March 2011.

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This report has been approved for public release.

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EVAPORATION DYNAMICS OF A SEVEN-COMPONENT MIXTURE CONTAINING NERVE AGENT SIMULANTS

1. INTRODUCTION

1.1 Background

Mixtures of chemicals found in the environment may or may not evaporate according to the well-known principles articulated in Raoult's Law for ideal solutions, that is, the volatility of each component in a mixture is the product of its single-component volatility (vapor pressure) and mole fraction. This work explores the evaporation rate of a seven-component mixture comprised of three volatile components and four non-volatile components. The three volatile components investigated were di-(n-propyl) ether (PE), dimethyl hydrogen phosphonate (DMHP), and dimethyl methylphosphonate (DMMP). These volatile components were investigated in order from highest to lowest vapor pressure.

The components of an ideal solution will have equilibrium partial pressure (p) given by the following equation:

$$\mathrm{P} = (p^*_{\mathrm{A}})\mathrm{x}_{\mathrm{A}} + (p^*_{\mathrm{B}})\mathrm{x}_{\mathrm{B}} = \cdots,$$

and the individual vapor pressure for each component is:

$$p_{\mathrm{i}} = (p^*_{\mathrm{i}})x_i$$

where

P is the total relative pressure of all vapor components, ideally 1.000
p_i is the partial pressure of the component i in the mixture
p^*_i is the equilibrium vapor pressure of pure component i
x_i is the mole fraction of component i in the liquid phase

Low-volatility components will suppress the partial pressure of the solution components in proportion to their mole fraction. Raoult's Law is valid only under the assumption that the chemicals form an ideal solution, and deviations, both negative and positive, are possible. Deviations from Raoult's Law may indicate the strength of interactions between components of a mixture in question[1].

1.2 Objective

In the following, we report the evaporation dynamics of a seven-component mixture as described in the experimental section below by quantifying the effluent vapor phase mixture. Mass balance equations are then used to infer the composition of the remaining liquid mixture. The measured data are compared to expectations based on the Raoult's Law predictions and what would be expected for pure (single-component) materials, which defines the maximum and minimum evaporation rates for materials that follow Raoult's Law or have positive

deviations. Negative deviations from Raoult's Law are also possible and would be manifested by evaporation rates that are slower than predicted.

2. EXPERIMENT

Vapor streams were generated by flowing inert carrier gas at a fixed rate through a saturator cell held in a water bath at a controlled temperature. Vapor pressure (for pure compounds) or partial pressure (for mixtures) may be inferred using the Ideal Gas Law[2]. If the ambient pressure and carrier flow rate are known the partial pressure of the exiting vapor can be determined at the bath temperature by quantifying the amount of analyte lost from the saturator. In the present work, exiting vapors are carried through a heated transfer line into the Dynatherm (CDS Analytical, LLC, Oxford, PA) trap then desorbed and transferred to a gas chromatograph (GC) equipped with a flame ionization detector (FID) where the mass of the analyte in that sample can be determined. In this work, a calibration curve was built using liquid injections through the GC inlet. GC area has been correlated to mass injected using standard procedures that have been described in detail elsewhere.[3]

Mass spectrometry and GC were used to identify and quantify, respectively, the analytes of interest. Analytical system operating parameters are provided in Appendix A.

In order to validate system operation, the experimental system was used to measure the vapor pressure of naphthalene. Those results are compared to literature values[3,4] and are provided in Appendix B.

Appendix C contains liquid injection calibration data for the three volatile components investigated in the present work.

System operation was validated by investigating the vapor pressure of DMMP and comparing those results to literature values[3]. Details of that work are provided in Appendix D.

A scoping experiment was performed using four of the components of interest, and a brief description of those results is provided in Appendix E.

Appendix F contains data measured for a second seven-component mixture, similar to the first. There were no significant differences observed for the two runs.

3. RESULTS AND DISCUSSION

Evaporation dynamics of a mixture comprised of seven components, as listed in Table 1, was determined in the present work.

Table 1. Seven-Component Mixture Composition

Compound	Target Mass Ratio to DMMP	Mass Needed for ~5-mL Volume (g)	Actual Mass* (g)	Mass Ratio to DMMP	Mole Ratio
Propyl ether	0.089	0.444	0.472	0.096	0.100
DMMP	1.000	5.000	4.922	1.000	0.859
DMHP	0.010	0.050	0.056	0.011	0.011
Pyro (04-0046-86)**	0.006	0.028	0.021	0.004	0.003
MPMA	0.028	0.140	0.138	0.028	0.015
MPAA (solid)	0.037	0.187	0.039	0.008	0.004
H_3PO_4	0.000	0.002	0.031	0.006	0.007

*Total saturator sample mass is 5.679g.
**This compound preparation was recorded in notebook number 04-0046-86.
H_3PO_4, phosphoric acid
MPAA, methylphosphonic acid anhydride trimer
MPMA, methyl methylphosphoric acid
Pyro, bis-dimethyl methyl phosphonate

The analytical system was calibrated for the volatile compounds by GC-FID. Volatile compounds measured include DMMP, DMHP, and PE. Non-volatile compounds used in this study were Pyro, MPMA, H_3PO_4 and MPAA. Helium was used as carrier gas.

After loading the saturator cell and a brief equilibration period, data collection commenced. Volatile compounds in the mixture were quantified as a function of time. The measured PE data are listed in Table 2. Those data were used to develop a time dependence for PE mass loss rate, shown in Figure 1. The mass loss rate, integrated over time, provides a measure of the amount of PE remaining in the saturator. The resulting correlation equation is shown in Figure 2, along with extremes anticipated for ideal mixture solution and pure PE component evaporation rates. Figure 2 shows that the experimental data yields an evaporation rate which has been suppressed by the presence of the other components, while the pure PE component yields the fastest mass loss rate possible for PE. The mass loss rate was corrected for Dynatherm efficiency by observing that the majority of PE had evaporated over the first 500 min of the test. Integration of the curve in Figure 1 indicates a mass loss of ~75% from the saturator at the time the experiment was terminated, mostly due to DMMP and non-volatile components remaining in the saturator.

Table 2. Corrected Propyl Ether Mass Collected During Two-Minute Collection Times at 30-Minute Intervals and Mass Loss Rate

Time (min)	FID Area (10^6)	PE Mass (μg)	Mass Loss Rate (μg/min)
1	8401.06	3847	1923
30	7884.19	3513	1757
60	7350.33	3178	1589
90	6046.79	2405	1202
120	4506.02	1580	790
150	3573.84	1135	567
180	3029.60	896	448
210	2622.21	729	364.5
240	2341.54	620	310.1
270	2095.75	529	264.6
390	1330.28	276	138.2
420	976.78	178	88.9

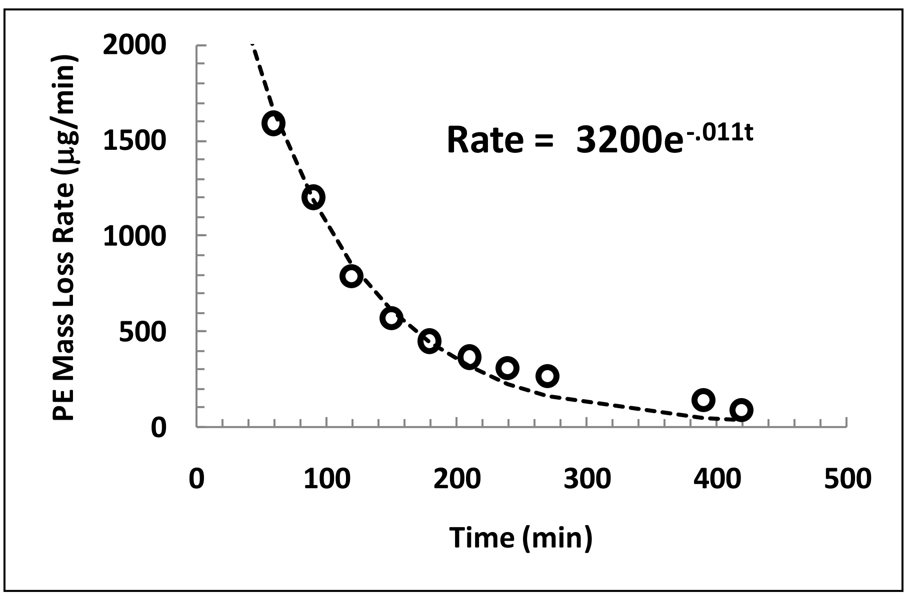

Figure 1. Propyl ether mass loss rate versus time and logarithmic correlation equation.

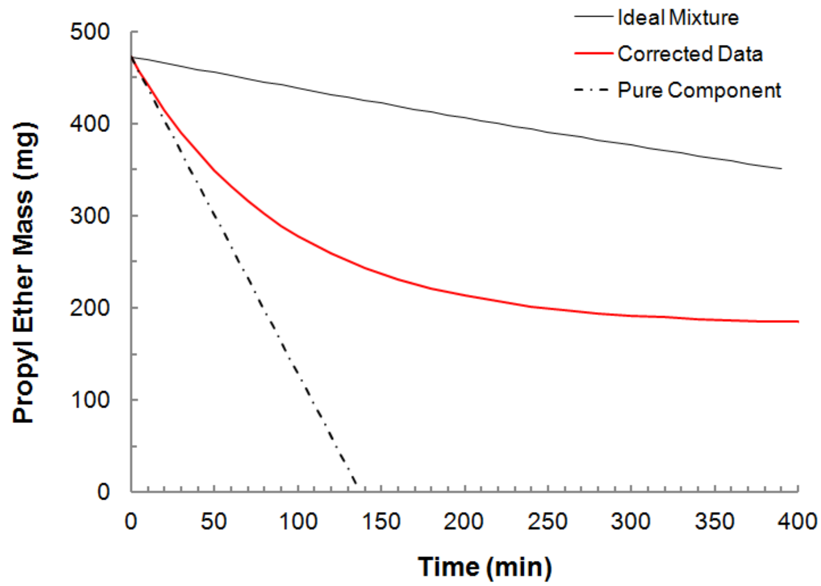

Figure 2. Corrected propyl ether mass versus time plot (red line) for seven-component mixture. Black line depicts the mass loss rate expected based on Raoult's Law, and the dash-dot line shows the expected mass loss from pure PE.

A similar analysis was performed for DMHP mass loss from the seven-component mixture. The experimental data are listed in Table 3. A plot of mass loss rate versus time is shown in Figure 3, along with the correlation equation derived from those data. A plot of mass versus time is provided in Figure 4. In this case, the observed mass loss rate is very close to what was expected based on Raoult's Law.

Table 3. DMHP Mass Observed During Two-Minute Collection Times at 30-Minute Intervals and Mass Loss Rate Data in Seven-Component Mixture Experiment

Time (min)	FID Area (10^6)	Mass (μg)	Mass Loss Rate (μg/min)
1	36.31	6.19	3.095
30	38.53	6.57	3.285
60	39.06	6.66	3.33
90	32.59	5.56	2.78
120	33.28	5.67	2.835
150	34.73	5.92	2.96
180	34.82	5.94	2.97
210	32.99	5.62	2.81
240	33.65	5.74	2.87
270	33.47	5.70	2.85
390	33.50	5.71	2.855
420	33.08	5.64	2.82
1220	30.89	5.27	0.635
1250	30.79	5.25	0.625
1280	30.31	5	2.5
1310	30.37	5	2.5
1340	30.22	5	2.5
1370	30.02	5	2.5
1400	29.92	5	2.5
1430	29.87	5	2.5
1460	29.83	5	2.5
1490	29.57	5	2.5
1520	29.39	5	2.5

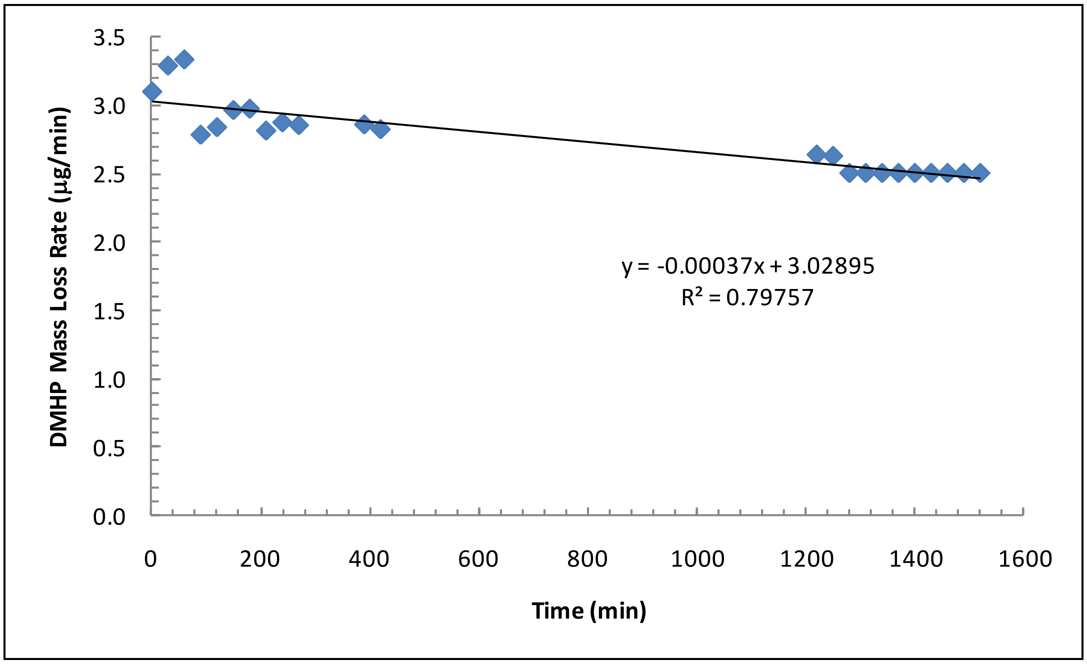

Figure 3. DMHP mass loss rate versus time and linear correlation equation.

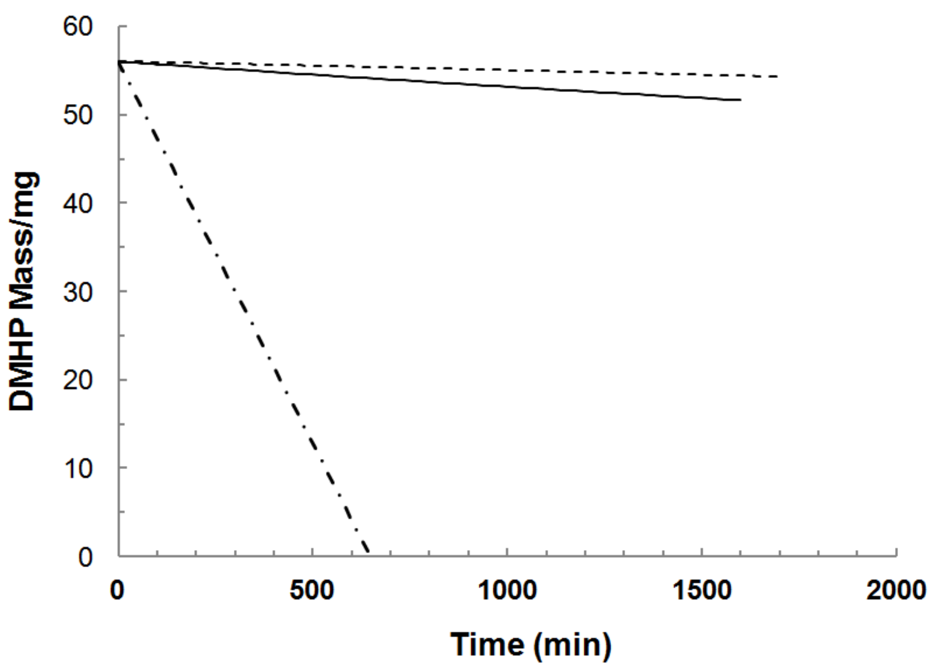

Figure 4. DMHP mass loss in seven-component mixture experiment (solid line), compared to ideal solution prediction (dashed line) and pure component (dash-dot line).

The experimental data for DMMP are listed in Table 4. The same analysis is not necessary since the DMMP behavior is less complicated. Excluding the first data point, the mass loss rate, shown in Figure 5, increases by about 15% to a maximum of approximately 55 μg/min. During the course of the experiment, total DMMP mass loss observed was approximately 1.2 g, and the inferred vapor pressure appears to be slightly less than, but within current experimental error limits, of the pure component value. The initial increase is caused by loss of PE, primarily, but also DMHP over the first several hours of the experiment. The steady state value corresponds to the value expected based on DMMP vapor pressure, but slightly reduced owing to the presence of the non-volatile components in the mixture. These results suggest that the DMMP and DMHP approximate an ideal solution, while PE is behaving less ideally.

Table 4. DMMP Mass Observed During Two-Minute Collection Times at 30-Minute Intervals and Mass Loss Rate Data in Seven-Component Mixture Experiment

Time (min)	FID Area (10^6)	Mass (μg)	Mass Loss Rate (μg/min)
1	644.25	78	39.0
30	765.17	93	46.5
60	804.95	98	49.0
90	821.49	100	50.0
120	827.24	101	50.5
150	834.37	102	51.0
180	839.7	102	51.0
210	843.52	103	51.5
240	853.97	104	52.0
270	854.92	104	52.0
390	861.67	105	52.5
420	861.63	105	52.5
1220	859.99	105	52.5
1250	867.73	106	53.0
1280	865.86	105	52.5
1310	867.25	106	53.0
1340	869.96	106	53.0
1370	870.91	106	53.0
1400	872.14	106	53.0
1430	873.74	106	53.0
1460	878.78	107	53.5
1490	875.62	107	53.5
1520	876.81	107	53.5

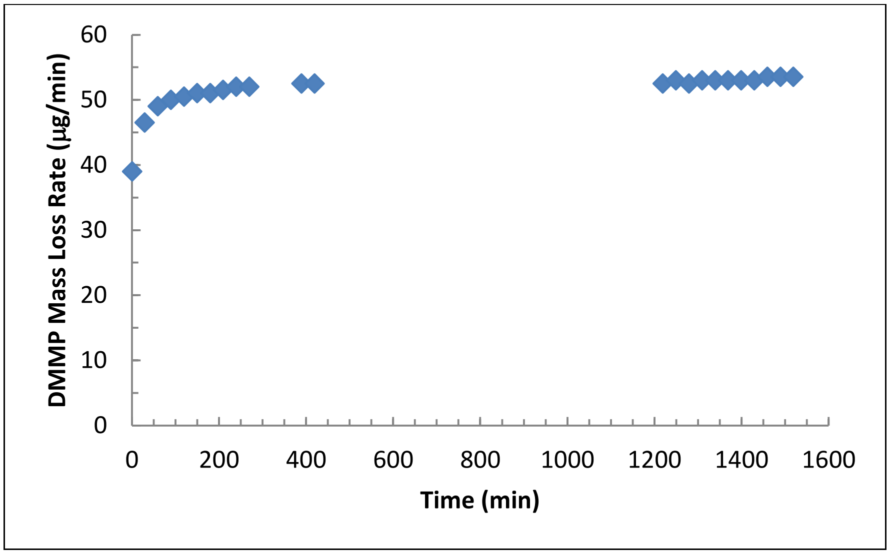

Figure 5. DMMP mass loss rate versus time.

A second seven-component mixture experiment was performed, and the results were similar to those described above. Details of that work are provided at Appendix F.

4. CONCLUSIONS

In the current work, PE evaporated initially at a rate approaching that of pure material, suggesting that it does not form an ideal solution with DMMP and DMHP. At later times, it appears to deviate from the non-ideal evaporation rate, that is, intermediate between what would be expected for pure PE and an ideal mixture. The measured data have been corrected for DynaTherm efficiency caused by saturation effects.

In the present work, DMHP and DMMP behaved nearly as predicted by Raoult's Law, particularly after depletion of the more volatile PE component. This result was expected owing to the similarity of these two materials. It is most likely that their slightly reduced volatility observed in the present work is due to the presence of the non-volatile components of the mixture.

The evaporation dynamics observed for the mixture used in the present work are not remarkable in any sense. Quantitative prediction of such data is not currently possible, and until such time that it is, empirical data is required to determine component evaporation rates.

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ACRONYMS AND ABBREVIATIONS

DMHP	dimethyl hydrogen phosphonate
DMMP	dimethyl methylphosphonate
ECBC	U.S. Army Edgewood Chemical Biological Center
FID	flame ionization detector
GC	gas chromatograph
H_3PO_4	phosphoric acid
MPAA	methylphosphonic acid anhydride trimer
MPMA	methyl methylphosphoric acid
MS	mass spectrometry
MSD	mass spectrometer detector
PE	di-(n-propyl) ether
Pyro	bis-dimethyl methyl phosphonate
RDECOM	U.S. Army Research, Development and Engineering Command
Rtx	Restek silica fused column
SCCM	standard cubic centimeters per minute
STD	standard
VP	vapor pressure

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APPENDIX A
ANALYTICAL SYSTEM PARAMETERS

The analytical system consisted of gas chromatographic interfaced to an autosampler for liquid injections with flame ionization and mass spectrometer detectors. The system also interfaced to the DynaTherm (CDS Analytical, LLC, Oxford, PA) sample collection delivery system and the saturator cell. Operating parameters for the hyphenated multi-component system are as follows:

1. GAS CHROMATOGRAPHER (GC)

Injection Parameters

Injection port: 200 °C	Injection mode: Splitless
Flow: 10.6 mL/min	Gas type: Helium

Oven Parameters

Initial temperature: 40 °C	Initial time: 0.5 min

Ramp: 5 °C/min to 80 °C and hold for 2 min, then 10 °C/min to 260 and hold for 5 min

Column

Restek Rtx 1701(fused silica) max temp 280 °C , nominal length 30.0 m, nominal diameter 530 µm, nominal film thickness 1µm
Initial pressure: 5 psi
Mode: Ramped pressure
Ramp: 0.70 psi/min, final pressure 6.90 psi, final time 7.50 min; 0.35 psi/min, final pressure 14.6 psi, final time 30 min

Flame Ionization Detector (FID) Parameters

Temperature: 250 °C
Hydrogen flow rate: 450 mL/min
Air flow rate: 450mL/min
Constant make up flow

Mass Spectrometer Detector (MSD) Transfer Line Heater

Initial temperature: 250 °C

2. MASS SPECTROMETER (MS)

Acquisition mode: SCAN

Scan range: 50 to 300 amu
MS source: 230 °C
MS quads: 150 °C

3. DYNATHERM PARAMETERS

Valve temperature: 103 °C
Tube temperature: 290 °C
Trap temperature: 300 °C
Heat time: 4 min
Dry time: 0 min
Ext time: 2 min
Trap time: 5 min

APPENDIX B
NAPHTHALENE VAPOR PRESSURE DATA

Before gas saturation measurements, system calibration and performance were tested using naphthalene, which has well documented vapor pressure data[5]. Only one temperature point was used for this verification process.

Calibration was performed for naphtalene, and the results are shown in Table B-1. The data and correlation are shown in Figure B-1.

Table B-1. Calibration Data for Naphthalene

Naphthalene Mass (µg)	FID Area ($\times 10^4$)	Volume Injected (µL)	Volume Used/Syringe Size (µL)	Calibration Solution Concentration (µg/mL)
0.980	2.090	1.0	1/1	980
0.980	1.933	1.0	1/1	980
0.980	1.987	1.0	1/2	980
1.960	3.916	2.0	2/2	980
1.960	3.967	2.0	2/2	980
2.940	5.806	3.0	3/5	980
1.960	3.799	2.0	2/5	980
0.980	1.769	1.0	1/5	980
1.960	3.785	2.0	2/5	980

FID, flame ionization detection

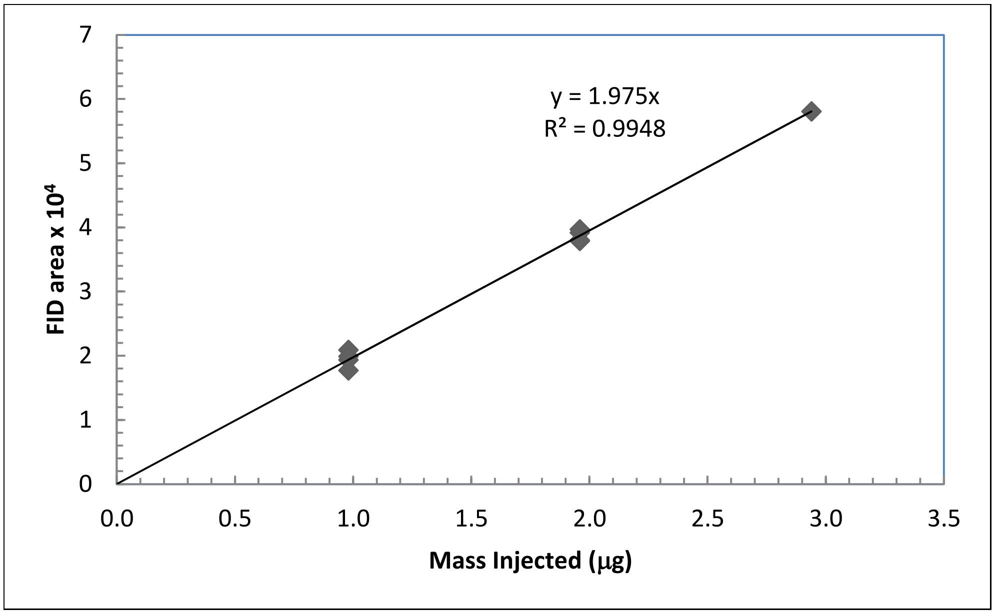

Figure B-1. Calibration curve for naphthalene from data listed in Table B-1.

After calibration, the gas saturation cell is operated to verify that data can be produced which agrees with literature values for the reference material (naphthalene). Table B-2 illustrates the measurements obtained from the calibrated system and the theoretical (literature) value. Percent difference is calculated to show variation between literature and experimental.

Table B-2. Naphthalene Vapor Pressure at 5 ºC Measured Using the Gas Saturation Technique[4]

Temp (°C)	Naphthalene Vapor Pressure (Pa)	Calculated Vapor Pressure (Pa)[4]	Percent Difference $100(P_{exp}-P_{calc})/P_{calc}$
5.0	1.39	1.35	2.75
5.0	1.39	1.35	2.64
5.0	1.39	1.35	2.89
5.0	1.39	1.35	2.62
5.0	1.39	1.35	2.65
5.0	1.39	1.35	2.87
5.0	1.39	1.35	3.31
5.0	1.39	1.35	2.70
5.0	1.39	1.35	2.66
5.0	1.39	1.35	2.71
5.0	1.39	1.35	3.15
5.0	1.39	1.35	2.88
5.0	1.39	1.35	2.72
5.0	1.38	1.35	2.29
5.0	1.39	1.35	2.83

APPENDIX C
DMMP, DMHP, AND PE CALIBRATION DATA

Calibration was performed for di-(n-propyl) ether (PE), and the results are shown in Table C-1. The data and correlation are shown in Figure C-1.

Table C-1. Calibration Data for PE

Standard Concentration (mg/mL)	Volume Injected (µL)	Mass Injected (µg)	FID Area (10^6)
15	1	15	528
15	2	30	1019
15	3	45	1507
15	4	60	1964
15	5	75	2288

FID, flame ionization detector

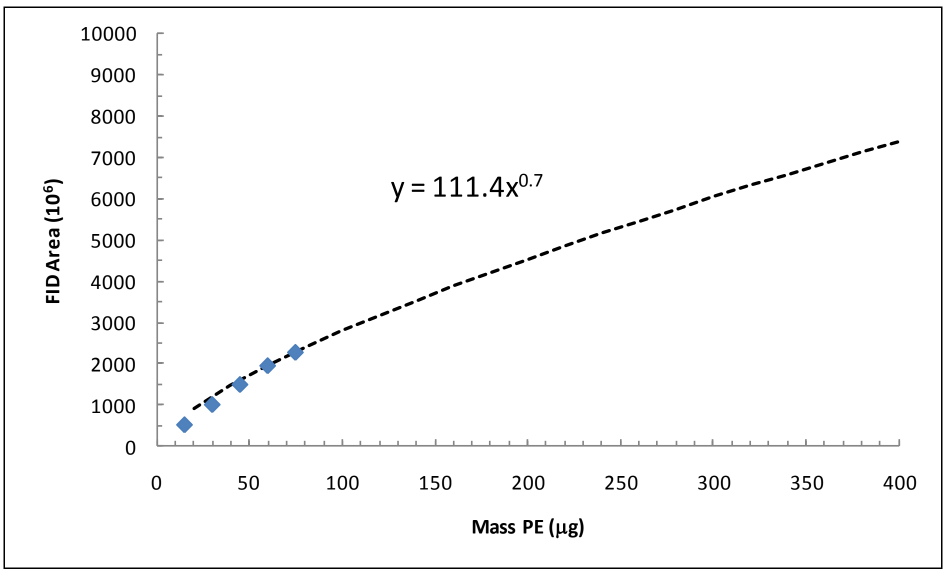

Figure C-1. Calibration curve for propyl ether.

A similar calibration was performed for dimethyl hydrogen phosphonate (DMHP), and the results are shown in Table C-2. The data and correlation are shown in Figure C-2.

Table C-2. FID Calibration Data for DMHP

Standard Concentration (mg/mL)	Injected Volume (μL)	Mass (μg) in column	DMHP area (10^6)
47.58	1	47.58	331.16
47.58	2	95.16	593.50
47.58	3	142.74	850.11
47.58	4	190.32	1101.02
47.58	5	237.9	1375.76

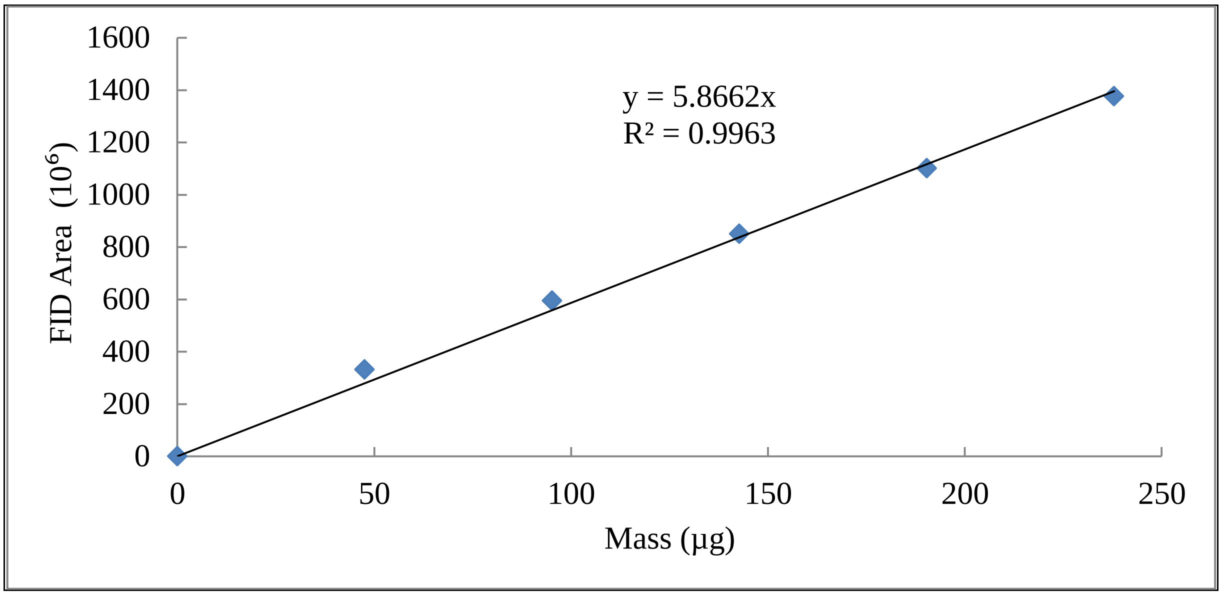

Figure C-2. Calibration curve for DMHP.

Table C-3. Calibration Data for DMMP

STD (mg/mL)	Injected Volume (μL)	Mass in column (μg)	Observed Peak Area × 10^6
22.85	1	22.8	221.84
22.85	2	45.7	392.39
22.85	3	68.5	539.34
56.84	1	56.8	491.61
56.84	2	113.7	935.21
56.84	3	170.5	1378.93

STD, standard

Calibration performed for dimethyl methylphosphonate (DMMP), the results data and correlation are shown in Table C-3 and Figure C-3.

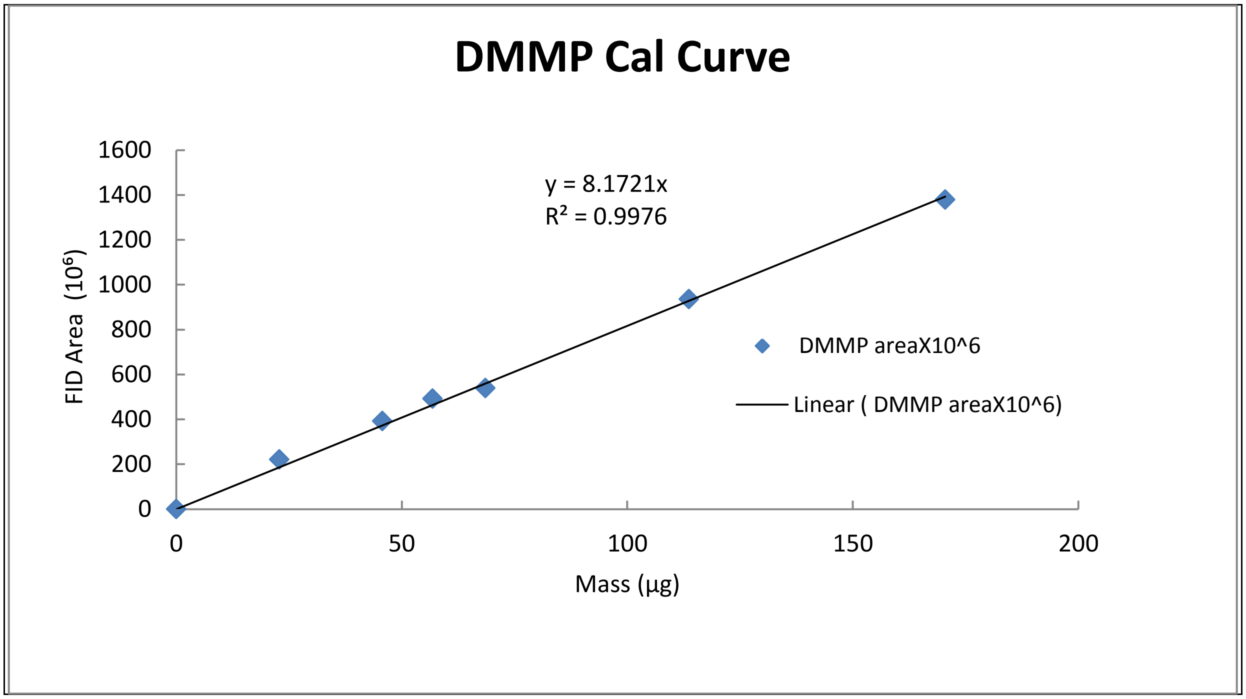

Figure C-3. DMMP calibration.

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APPENDIX D
DMMP VAPOR PRESSURE DETERMINATION

After calibration, dimethyl methylphosphonate (DMMP) (99% purity) vapor pressure at 15 °C was determined using the gas saturation method. The data is presented (Table D-1) which is also the temperature used for the seven-component mixture determination. This data is a baseline and will be compared against mixture data to observe any changes in vapor composition with time. The measured flow rate was 14.8 standard cubic centimeters per min (sccm) through the saturator cell.

Table D-1. DMMP Vapor Pressure Measurement at 15 °C

Time (min)	DMMP Area (10^6)	DMMP Mass (μg)	VP DMMP (Pa)
1	898.6	110	73.7
37	904.1	111	74.1
67	893.5	109	73.3
94	897.0	110	73.5
121	897.0	110	73.5
148	898.5	110	73.7
175	905.4	111	74.2
202	904.2	111	74.1
229	909.4	111	74.6
255	911.5	112	74.7
297	909.4	111	74.6
318	913.8	112	74.9
339	913.0	112	74.8

VP, vapor pressure

The vapor pressure of pure DMMP (99%) was measured using the method described above. The results are compared to data previously reported[2]. Four temperatures (5 °C, 10 °C, 15 °C, and 20 °C were compared to Buchanan’s correlation as shown in Appendix E.

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APPENDIX E
FOUR-COMPONENT MIXTURE DMMP VAPOR PRESSURE

Dimethyl methylphosphonate (DMMP) calibration was performed prior to operation of the saturator cell as a positive control and to investigate detector response. DMMP vapor pressure data using gas saturation was performed at temperatures of 5, 10, 15, and 20 ºC. Results are compiled in Table E-1. Figure E-1 is the corresponding vapor pressure graph showing our DMMP data compared to the correlation recently published by Buchanan et al.[2] The slight increase over time observed in the four-component experiment, shown in Figure E-2, is likely caused by the loss of di-(n-propyl) ether (PE) during the first 300–400 min of that experiment.

Table E-1. DMMP Vapor Pressure Data Measured Using the Gas Saturation Technique

Temp (°C)	Number of Data Points	Average VP (Pa)	Antoine Equation VP (Pa)	% Difference $100(P_{exp}-P_{calc})/P_{calc}$	Standard Deviation
5.0	7	24.09	23.46	2.69	0.067
10.0	15	35.99	35.49	1.41	0.107
15.0	22	51.91	52.76	-1.61	0.215
20.0	17	71.95	77.16	-6.75	0.243

VP, vapor pressure

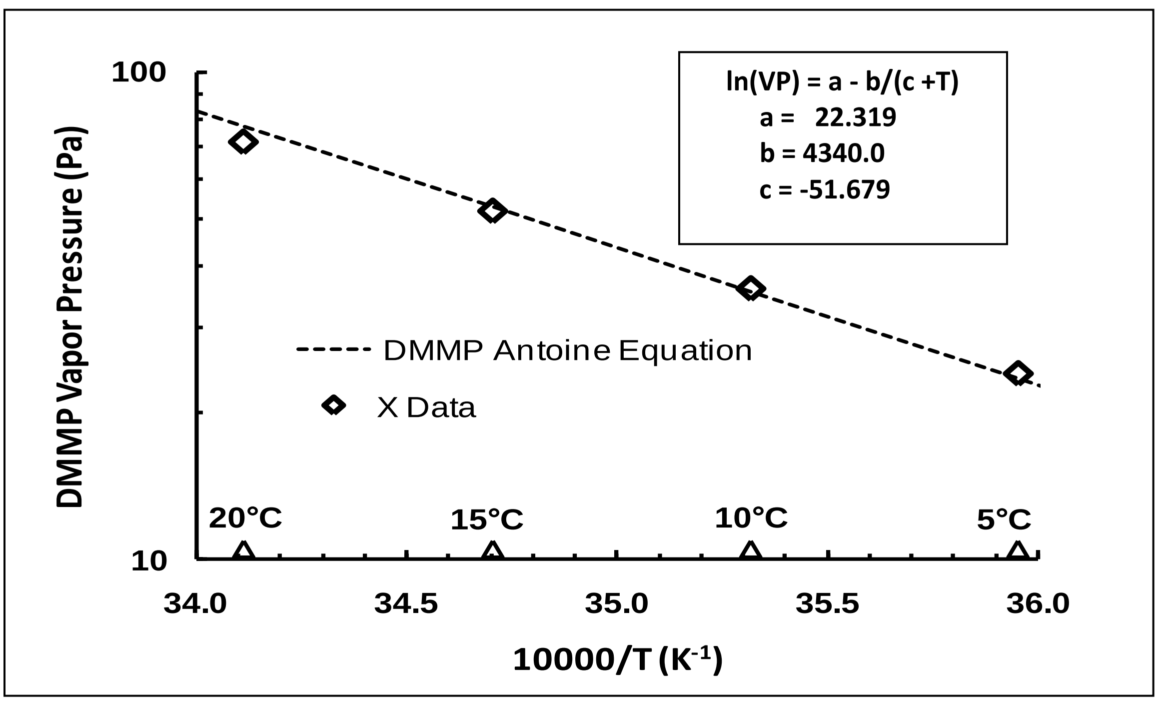

Figure E-1. DMMP vapor pressure curve illustrating agreement between this work and Antoine Equation of Buchanan et al.

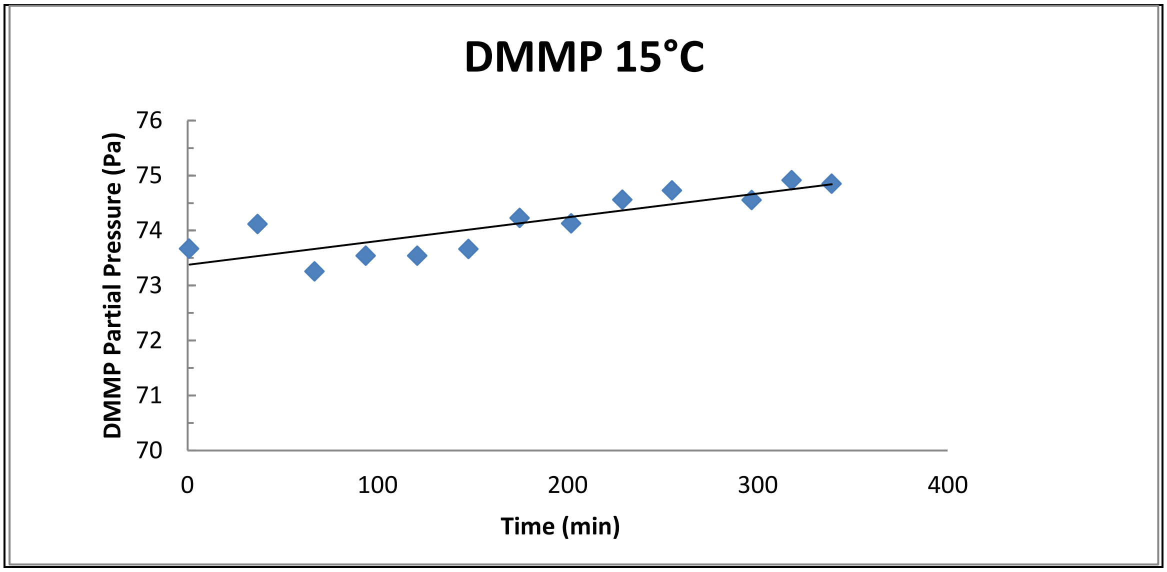

Figure E-2. DMMP partial pressure versus time in preliminary four-component experiment.

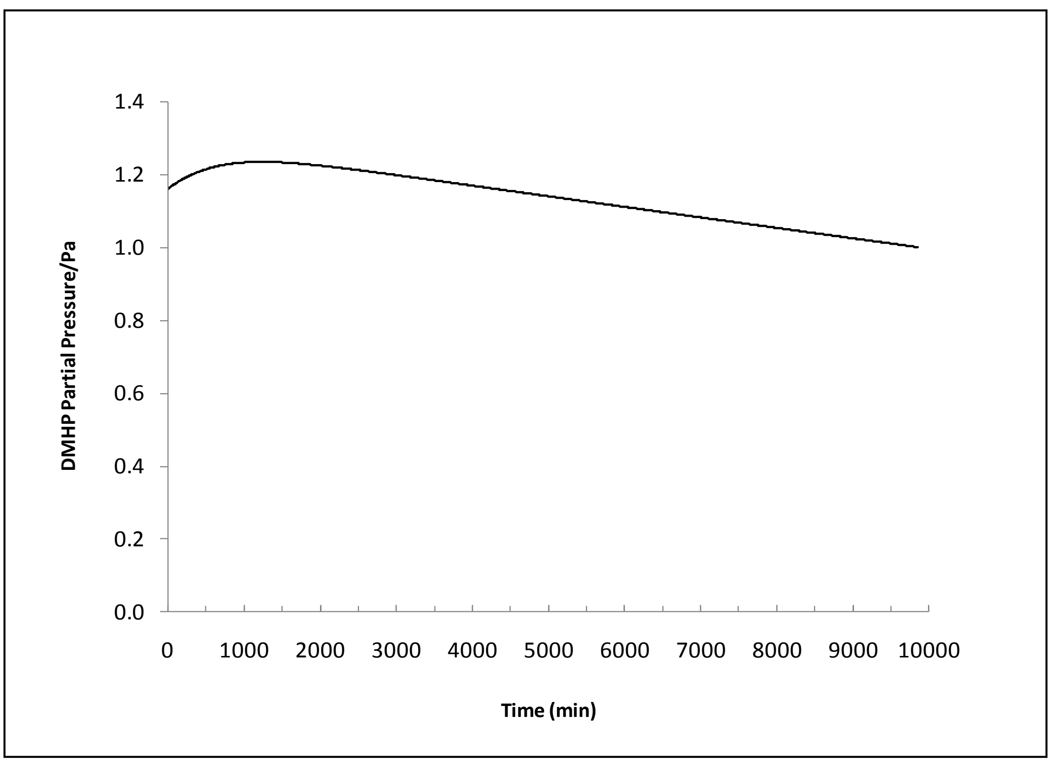

Figure E-3. Calculated partial pressure for dimethyl hydrogen phosphonate (DMHP) in four-component mixture.

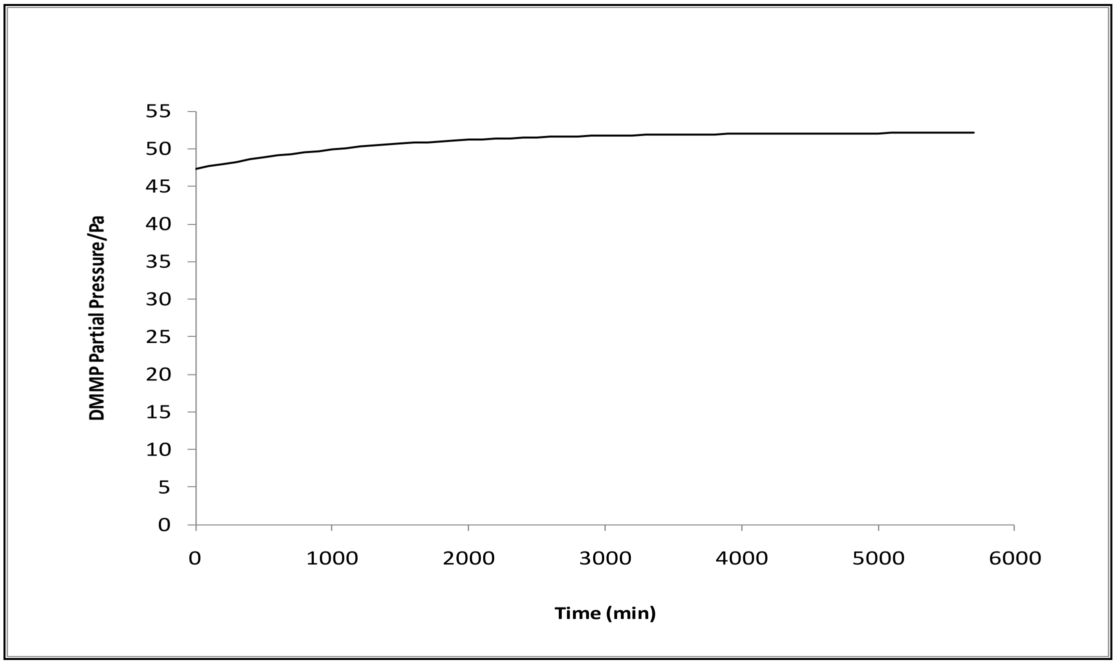

Figure E-4. Calculated partial pressure for DMMP in four-component mixture.

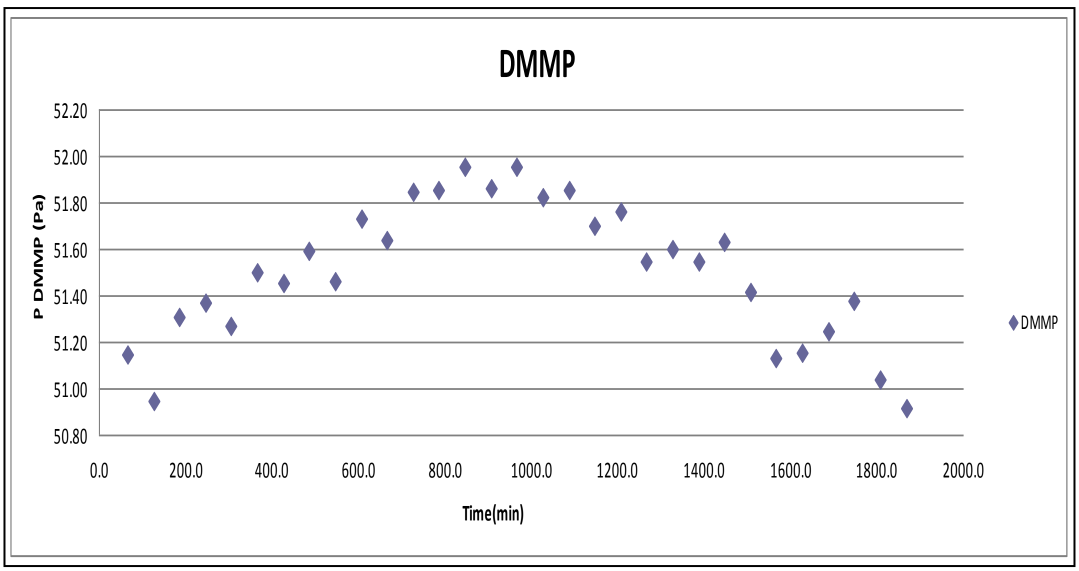

Figure E-5. DMMP partial pressure (Pa) versus time for four-component mixture.

Table E-2. Propyl Ether, Gas Chromatograph (GC) Area Counts Observed at 15 ºC Using the Gas Saturation Technique

Time	PE Peak at 4.976
66.05	1065988
126.08	617042
186.1	421550
246.11	249743
306.13	90642
366.15	29830
426.18	10976
486.2	4332.4
546.22	1770.1
606.24	748.6
666.26	323.9

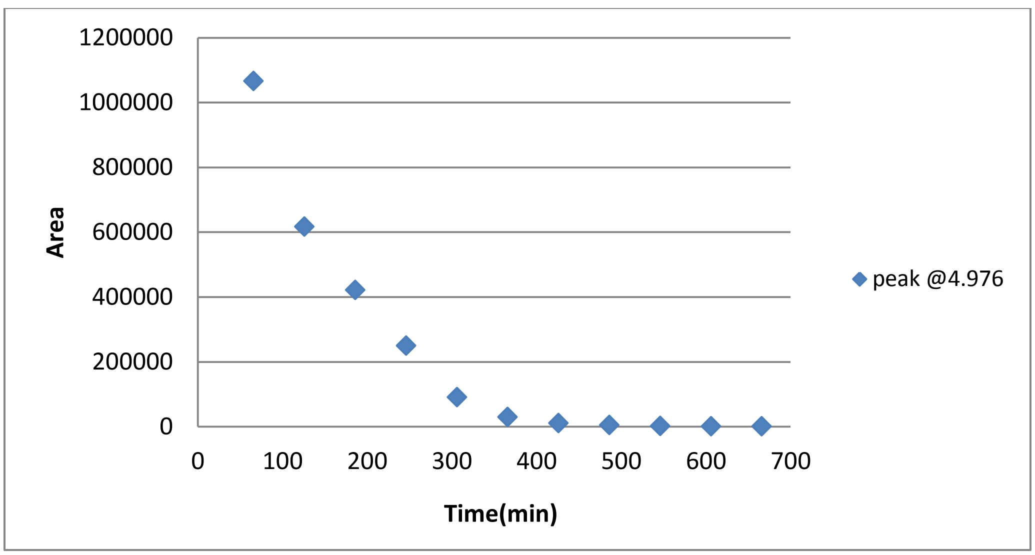

Figure E-6. Propyl ether partial pressure at 15 °C versus time for the four-component mixture experiment.

Table E-3. Measured DMHP Area at 15 ºC in Four-Component Mixture

Time	DMHP Area
66.05	13377.9
126.08	13428
186.1	13524.2
246.11	13436.7
306.13	13529.4
366.15	13510.9
426.18	13515.8
486.2	13488.2
546.22	13496.1
606.24	13485.8
666.26	13431.8
726.28	13468.8
786.31	13463.1
846.34	13477.1
906.37	13390.7
966.4	13396.3
1026.43	13368.1
1086.45	13335.8
1146.49	13319.7
1206.51	13286
1266.54	13248.3
1326.57	13257.4
1386.6	13201.1
1446.63	13187.3
1506.66	13155
1566.68	13075.1
1626.71	13042.4
1686.73	13055.1
1746.76	13042.1
1806.78	12996.7
1866.81	12896.3

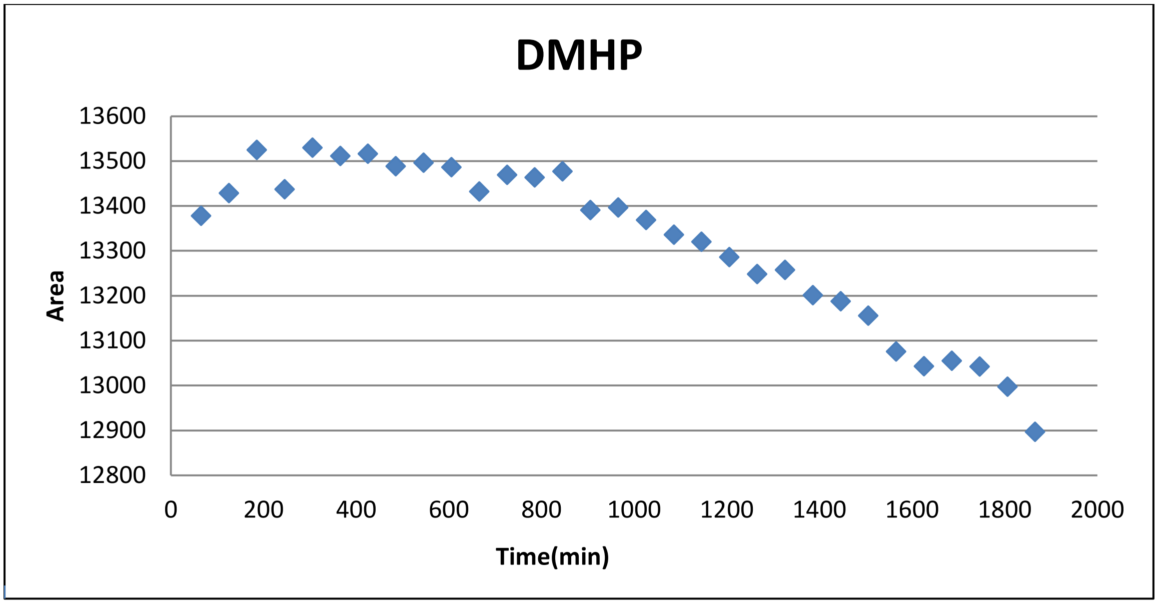

Figure E-7. DMHP at 15 ºC vapor measured, plotted area versus time for four-component mixture.

APPENDIX F
SUMMARY OF SECOND SEVEN-COMPONENT MIXTURE DATA

Table F-1. Second Seven-Component Mixture Composition

Compound	Target Ratio to DMMP	Measured Mass (g)	Actual Ratio to DMMP
Propyl Ether	0.089	0.445	0.089
DMMP	1.000	5.000	1.000
DMHP	0.010	0.413	0.083
Pyro	0.006	0.034	0.007
MPMA	0.028	0.169	0.034
MPAA	0.037	0.193	0.039
H_3PO_4	0.000	0.022	0.004

DMHP, dimethyl hydrogen phosphonate
DMMP, dimethyl methylphosphonate
$H3PO_4$, phosphoric acid
MPAA, methylphosphonic acid anhydride trimer
MPMA, methyl methylphosphoric acid
Pyro, bis-dimethyl methyl phosphonate

Table F-2. DMMP Mass Observed During Two-Minute Collections at 30-Minute Intervals in the Second Seven-Component Mixture Experiment

Time (min)	FID Area (10^6)	Mass (μg)	DMMP Partial Pressure (Pa)
1	721.40	88	58.7
30	804.50	98	65.5
60	835.97	102	68.1
90	842.01	103	68.6
120	849.90	103	69.2
150	848.15	103	69.1
180	851.03	104	69.4
210	853.93	104	69.6
240	854.38	104	69.6
270	854.22	104	69.6
300	856.34	104	69.8
330	857.07	104	69.9
360	856.09	104	69.8
390	857.43	104	69.9
420	860.56	105	70.2
450	863.21	105	70.4
1440	836.61	102	68.2
1470	839.56	102	68.5

FID, flame ionization detector

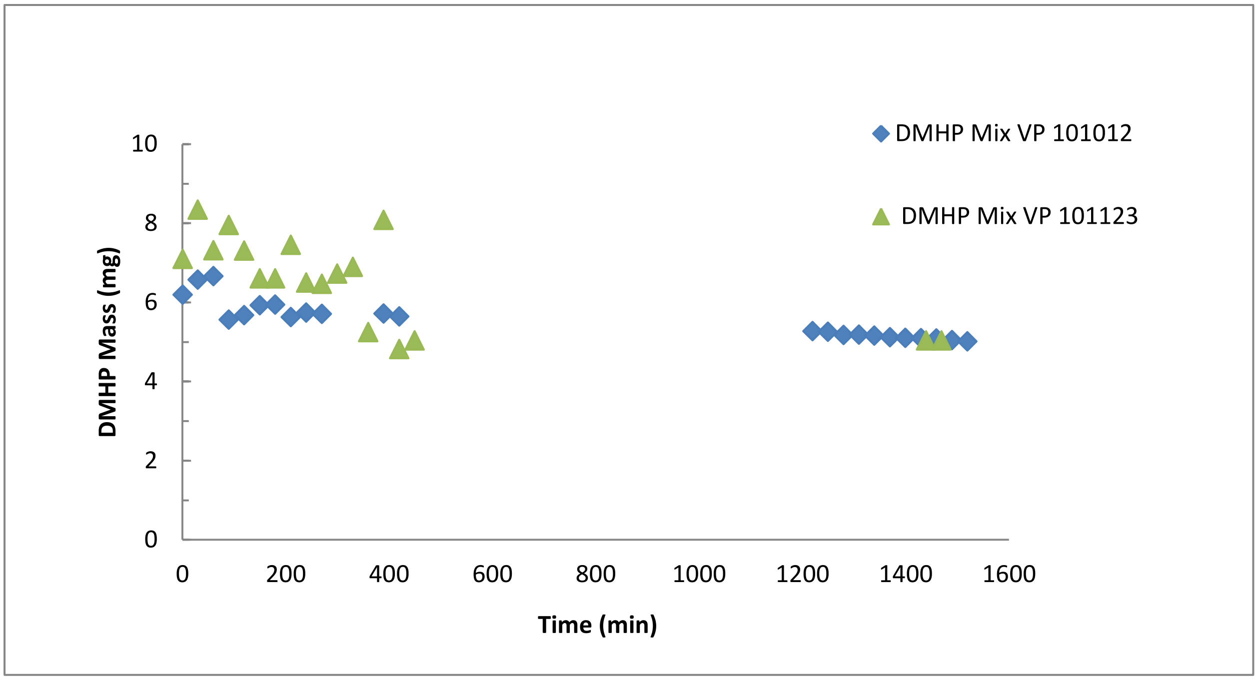

Figure F-1. DMHP mass in seven-component mixture versus time.

Table F-3. DMHP Amount in Mixture 2 Measured as Evolved from Mixture

Time (min)	Temp (°C)	DMHP MS Area (10^6)	DMHP Mass (µg)
1	15.0	8222.33	257
30	15.0	7640.00	239
60	15.0	6902.15	216
90	15.0	5423.79	170
120	15.0	4141.12	129
150	15.0	3409.07	107
180	15.0	2892.13	90
210	15.0	2517.59	79
240	15.0	2210.01	69
270	15.0	1945.81	61
300	15.0	1759.40	55
330	15.0	1482.92	46
360	15.0	1010.06	32
390	15.0	700.20	22
420	15.0	462.30	14
450	15.0	358.26	11

MS, mass spectrometer

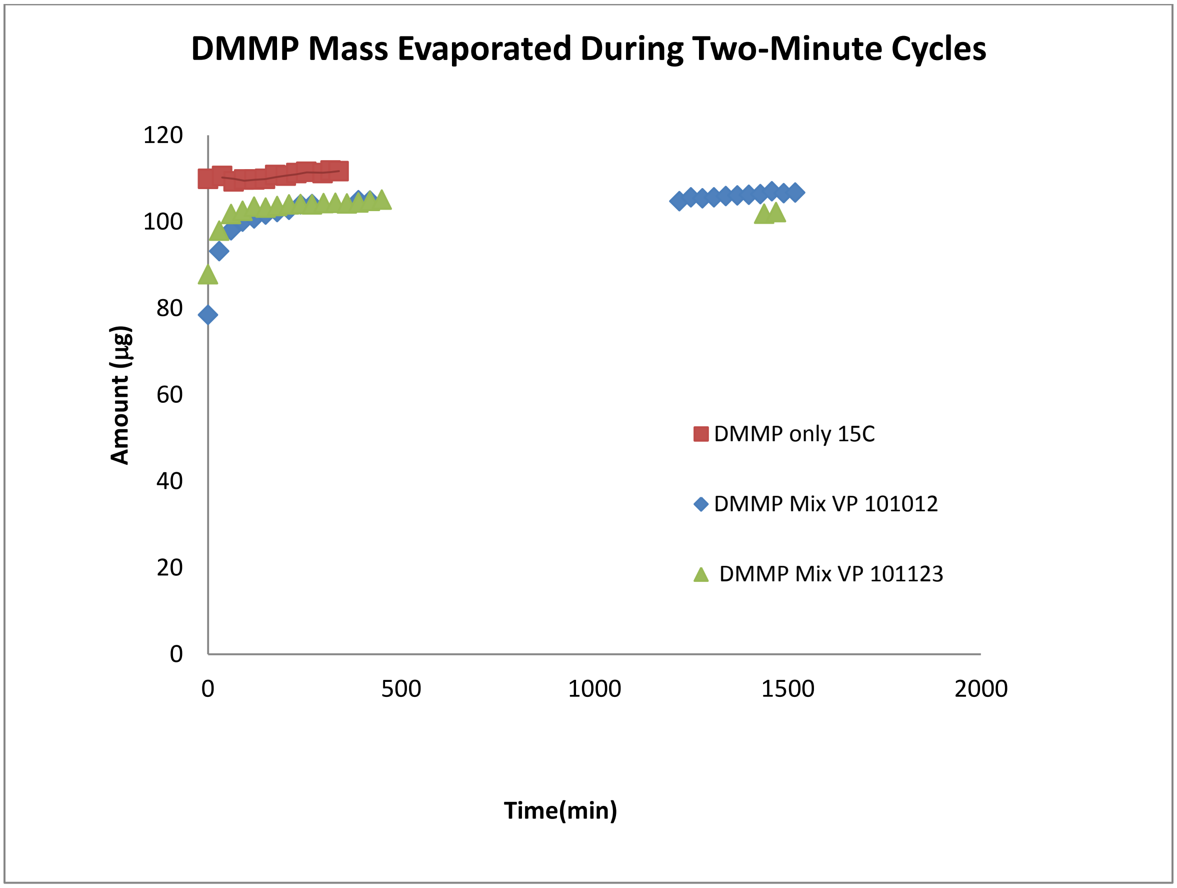

Figure F-2. DMMP two-minute mass loss versus time for mixtures 1 and 2 overlaid with pure DMMP mass loss data.

Table F-4. Seven-Component Mixture Propyl Ether Data

Time (min)	Propyl Ether MS Area (10^6)	Propyl Ether Mass (µg)	PE Partial Pressure (Pa)
1	8222.33	257	208.65
30	7640.00	239	193.88
60	6902.15	216	175.19
90	5423.79	170	137.71
120	4141.12	129	105.18
150	3409.07	107	86.60
180	2892.13	90	73.48
210	2517.59	79	63.97
240	2210.01	69	56.16
270	1945.81	61	49.45
300	1759.40	55	44.71
330	1482.92	46	37.69
360	1010.06	32	25.67
390	700.20	22	17.80
420	462.30	14	11.75
450	358.26	11	9.11

PE, di-(n-propyl) ether

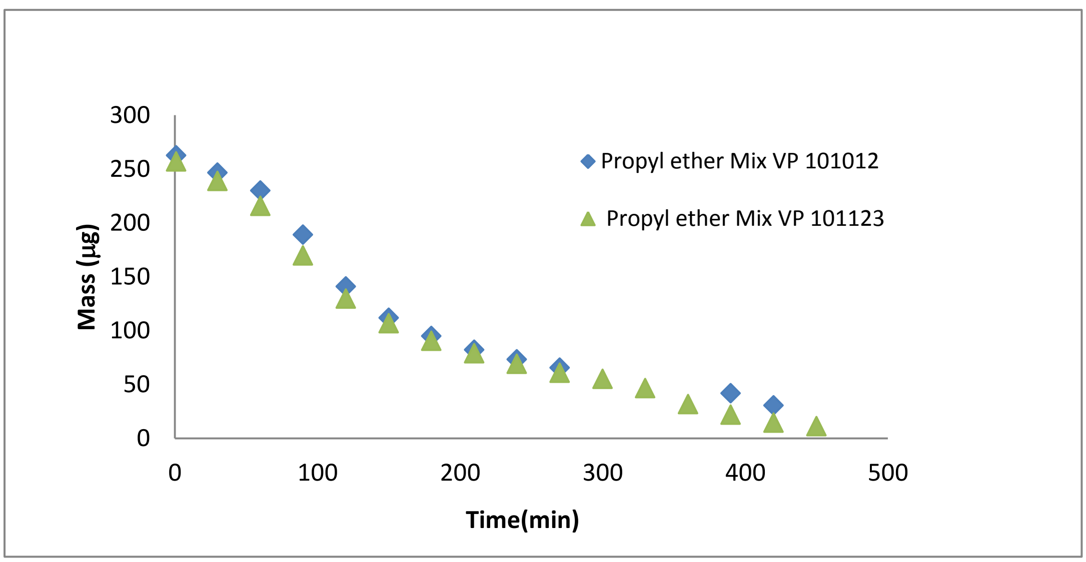

Figure F-3. Overlay for mixture 1 and 2 PE mass.

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